

Non-Equilibrium Molecular Dynamics Simulation of Electromigration in Aluminum-Based Metallic Interconnects

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Received 25.08.2006

Abstract

The effect of alloying elements in aluminum on diffusion behavior was investigated using non-equilibrium molecular dynamics (NEMD) under the effect of electromigration wind force. The electromigration wind force was computed based on a theory using the pseudopotential formalism of the elements, where it depends on the type and distribution of the imperfections in the lattice. It was found that the electromigration force on the impurity depends on the scattering power of the atom, which is related to the chemical valence. Elements like Cu, Li and Na gave low values, but the incorporation of such forces into molecular dynamics simulations underline the importance of the electromigration force distribution on the host aluminum atoms. In this regard, in NEMD formalism, we calculated the atomic jump frequency of aluminum atoms in alloys containing different impurity elements like Cu, Mg, Mn, Na, Sn and Ti. It was found that the electromigration diffusion process slowed down considerably, compared to pure Al, in alloys containing elements having a softer Al-M pair potential, namely Cu, Mn and Sn.

Key words: Electromigration, Diffusion, Non-equilibrium molecular dynamics.

Introduction

With the continuing miniaturization of integrated circuits, the electric current densities experienced in metallic interconnects in electronic circuits have multiplied. The consequence of such high current densities is the enhanced mass transport of atoms due to the momentum transfer between conducting electrons and diffusing atoms. This phenomenon is named electromigration and it plays a major role in the failure of interconnects due to vacancy diffusion induced void formation and growth occurring especially at grain boundaries. Aluminum has been widely used in such applications although it is not the perfect choice because of its fast diffusion kinetics. Therefore, very intensive research has been carried out to improve the properties of Al in terms of its resistance to electromigration, such as by adding small percentages of alloying elements like copper (Lloyd, 2002).

In addition, from the physics point of view, many theories have been developed to understand the phenomena with a deeper insight, and a recent summarized all the advances in the physics of electromigration (Sorbello, 1997). The phenomena were also reviewed from the aspects of thermodynamics and kinetics by Ho and Kwok (1989). Electromigration is basically a diffusion process under a driving force. In the literature, there are some phenomenological and theoretical approaches for the determination of this driving force (Sorbello, 1997). Moreover, in the last decade several computer simulations of electromigration in metal lines have been reported from the macroscopic point of view (Fridline and Bower, 1999; Arzt et al., 2001; Oğurtani and Oren, 2001).

It was found that the electromigration driving force is related to the direction of motion of the electrons and it is composed of 2 parts: the force from the applied electric field and the electron wind

force due to scattering. Fiks (1959) and Huntington and Grone (1961) formulated the electron wind force using a ballistic approach to handle the collision of electrons with the atoms. Huntington and Grone found that the driving force depends on the atomic configuration of the diffusion path and the types of the defects in the atomic structure. However, there is the problem of separating the systems of atoms, lattice and electrons in this method (Sorbello, 1972). A quantum-mechanical model was established by Bosvieux and Friedel (1961), in which the electron scattering force is taken as the electrostatic force of the electron charge acting on the scattering center using weak electron-ion Coulomb potentials. Then Sorbello (1972, 1980) and Kumar and Sorbello (1975) carried out very comprehensive studies, based on the pseudopotential description of the atoms, on determining the driving force for electromigration for each individual atom in the lattice. They studied the atomic configuration-dependent electromigration force including impurities of substitutional or interstitial kind and vacancies.

There are very limited studies in the literature involving atomistic simulations. A molecular dynamics (MD) study of electromigration was carried out by Ohkubo et al. (1996), where H type periodic boundaries for interconnects were constructed and two-dimensional MD simulations were carried out for aluminum. In that study the electromigration driving force was calculated using the Cloud in Cell (CIC) method and an evolution of void formation was reported. Shinzawa and Ohta (1998) characterized the grain boundary diffusion for aluminum interconnects by MD, where the diffusion characteristics with respect to the grain boundary angle were reported. Maroudas and Gungor (2002) studied the void evolution and failure in metallic thin films. In that study plastic deformations in the vicinity of the voids were examined by the use of MD.

In the present study, the effect of alloying elements in aluminum on diffusion behavior was investigated at different temperatures, using non-equilibrium MD under the effect of electromigration wind force. The electromigration wind force on each atom was determined by the use of a pseudopotential method described by Sorbello (1972). The investigated alloying elements include Cu, Mg, Mn, Na, Sn and Ti.

Computational Method

MD is based on the solutions of Newton's equations of motion for every atom making up the system where all are interacting via a potential. Time integration then gives the trajectories of the atoms from the forces calculated from interatomic interactions. Classical statistical mechanical concepts are then used to obtain the correspondence of the simulated system to a thermodynamic system.

In the present study, the atomic interactions were evaluated by a model potential approach. In this approach the effective pair potential between same types of atoms separated by a distance r is expressed as

$$V(r) = \frac{Z^2 e^2}{r} \left\{ 1 - \frac{2}{\pi} \int_0^{\infty} dq \left[1 - \frac{1}{\varepsilon} \right] M^2(q) \frac{\sin(qr)}{qr} \right\}$$

$$M^2(q) = \left[\frac{\Omega q^2}{4\pi e^2} \right] |W_0(q)|^2 \quad (1)$$

where M is the wavenumber characteristics, Z is the electronic charge of the atom, Ω is the atomic volume, q is the Fourier space vector, ε is the Hartree dielectric function and W_0 is the bare ion pseudopotential form factor, where for the evaluation of the form factors of elements used the technique and the parameters given by Heine and Abarenkov and Animalu (Heine and Abarenkov, 1964; Abarenkov and Heine 1965; Animalu, 1973) were adopted. In the calculation of the Hartree dielectric function, for its use in the screening of the bare ion potential, the local correction factor of the electron – electron interaction from Geldart and Vosko (1966) was used. The obtained pair potential for Al, given in Figure 1 together with other pair potentials, was tested for goodness with the General Utility Lattice Program (GULP) (Gale and Rohl, 2003) software, where the simulated lattice energy, the elastic constants, C_{11} and C_{12} and the lattice parameter in the face centered cubic (FCC) structure were compared with the experimental values as shown in Table 1. As can be seen, the derived potential predicts the experimental lattice parameter with an exceptional 3% error, which sometimes may not be obtained even by ab initio methods. In addition, the agreement in the lattice energy is fairly good. However, there is a discrepancy in the elastic constants, but it is not so dramatic, keeping in mind that pair potentials generally overestimate the elastic modulus because of the lack of many body interactions, if they were not specifically fitted to experimental modulus data.

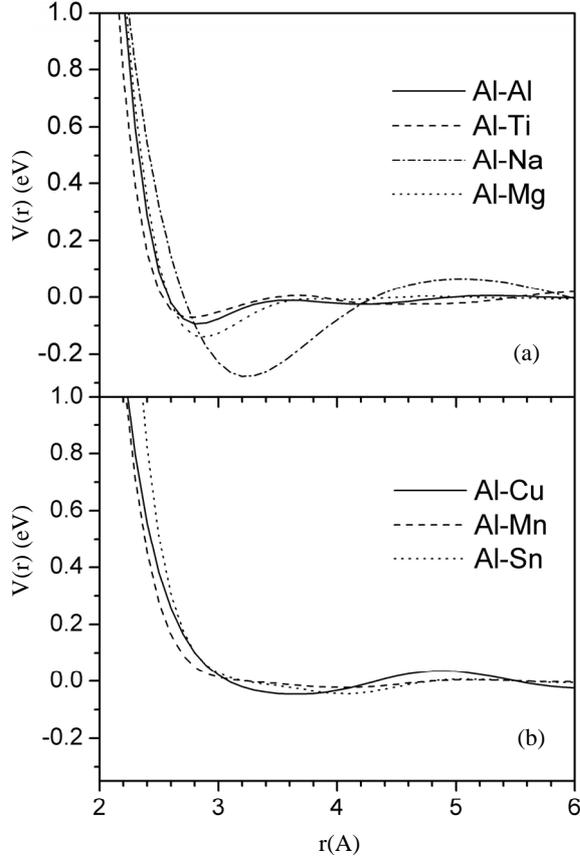


Figure 1. Computed interatomic pair potentials of Al-Al and Al-M ($M=\text{Cu, Mg, Mn, Na, Sn}$ and Ti) used in this study. Potentials of harder and softer nature were given in (a) and in (b), respectively.

Table 1. Properties of aluminum in the FCC structure using the computed interatomic potential in this study. Experimental data are from * (Bandyopadhyay and Gupta, 1978), † (Kittel, 1986), ‡ (Simmons and Wang, 1971).

Property	Calculated	Experimental
Lattice parameter (Å)	3.9300	4.0496*
Lattice Energy (eV)	-2.8189	-3.3983†
C_{11} (10^{11} dyne/cm ²)	22.396	10.649‡
C_{12} (10^{11} dyne/cm ²)	8.704	5.988‡

In the electromigration simulations, 8000 Al atoms were put into a $40.5 \times 81 \times 40.5$ Å MD box where there are actually $10 \times 20 \times 10$ unit cells of FCC lattice along the x , y and z Cartesian coordinates as schematically shown in Figure 2. In order

to observe the diffusion behavior under electromigration force, an electric field is applied along the positive x -axis direction. As a consequence of the electromigration force developed, the entire MD box moved along the same direction, which is not possible in the real system because of the boundary conditions imposed. In order to avoid this convective MD box motion, one unit cell from the top and one unit cell from the bottom along the y -axis were fixed. This results in 800 atoms being fixed: 400 from the top and 400 from the bottom. The introduction of the fixed atoms in the simulation box, however, hinders the motion of atoms that are nearby, which in effect enforces a reduction in the diffusion kinetics. In order to overcome this falsifying effect on the diffusion behavior, a rather larger simulation cell was constructed along the y direction and only the atoms placed in the middle of the box (system region composed of 4000 atoms) were analyzed for the determination of the diffusion properties. In order to introduce necessary vacancy defects, 32 atoms were taken out from this region. Additionally substitutional impurities such as Cu, Mg, Mn, Na, Sn and Ti atoms were placed here as well.

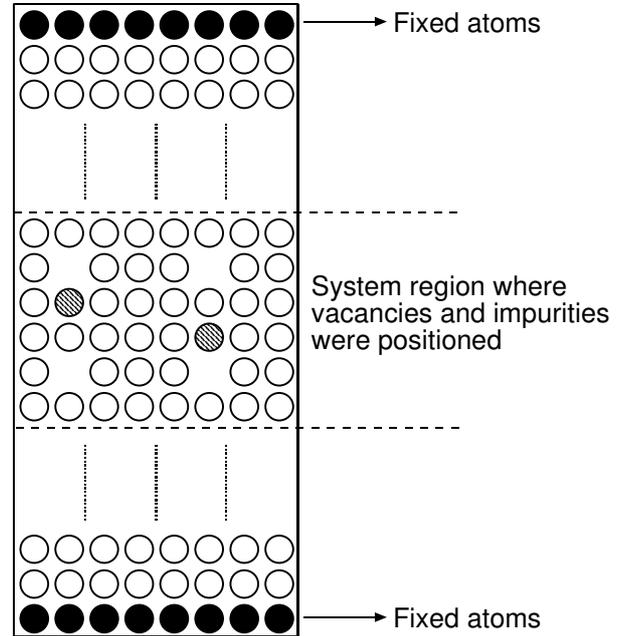


Figure 2. Schematic diagram of MD cell in 2 dimensions representing the distribution of host, fixed and impurity atoms and vacancies.

The electromigration force was calculated by the use of the pseudopotential approach described by

Sorbello (1972), where the electromigration force on an atom j due to an applied electric field depends on the impurities and vacancies in the lattice. Sorbello (1972) expressed the electron scattering force on an ion j in terms of potential U as

$$F_j = -\frac{\partial U_j}{\partial R_j}$$

$$U_j = - \sum_{\substack{n \\ \text{vacancies}}} u_{jn} + \sum_{\substack{i \\ \text{impurities}}} u_{ji} \quad (2)$$

where u_{jk} has to be defined for all of the possible cases of pair interactions. The possible pairs and their contribution to the potential in the calculation of electromigration force on the j^{th} atom are given in Table 2, where m is the atomic mass, R is the position vector, W is the screened pseudopotential form factor, $k_F = \left(\frac{3\pi^3 Z}{\Omega}\right)^{1/3}$ is the Fermi wave vector, ν_d is the electron drift velocity, ν_F is the Fermi velocity

and j_1 is the first order Bessel function of the first kind. In the force calculations, electron drift velocity of 0.01 a.u. was used. The calculated electromigration force was then added to the force obtained from the interatomic interactions and continued with the integration of the equation of motion in molecular dynamics. This added force perturbs the system that causes non-equilibrium conditions to be imposed, resulting in a continuous increase in the temperature. Thus, in order to keep the temperature constant, the system was coupled to a heat bath as described in the literature (Nose, 1984; Hoover, 1985) for thermostating. Then the integration of the motion of atoms was accomplished by the velocity Verlet integrator using a time step of 2 fs. Simulations were carried out in the canonical (NVT) ensemble at temperatures of 1000, 1200 and 1400 K, compared with the calculated melting temperature of 1800 K using the obtained pair potential for Al.

Table 2. Possible pairs for the calculation of the electromigration force acting on atom j .

Pairs		u_{jk} , for $k \leq N_{atom}$
Host	Host	0
Host $W_j \leftarrow \text{host}$ $R_j \leftarrow \text{host}$	Impurity $W_k \leftarrow \text{impurity}$ $R_k \leftarrow \text{impurity}$	$= u_{jk} + \left\{ -\frac{\Omega^2 m k_F}{4\pi^2 \hbar^2} \left(\frac{\nu_d}{\nu_F}\right) \cos(\nu_d, R_j - R_k) \times \int_0^{2k_F} W_j(q) [W_k(q) - W_j(q)] q^2 j_1(q R_j - R_k) dq \right\}$
Host $W_j \leftarrow \text{host}$ $R_j \leftarrow \text{host}$	Vacancy $R_k \leftarrow \text{vacancy}$	$= u_{jk} - \left\{ -\frac{\Omega^2 m k_F}{4\pi^2 \hbar^2} \left(\frac{\nu_d}{\nu_F}\right) \cos(\nu_d, R_j - R_k) \times \int_0^{2k_F} W_j(q)^2 q^2 j_1(q R_j - R_k) dq \right\}$
Impurity	Host	0
Impurity $W_j \leftarrow \text{impurity}$ $R_j \leftarrow \text{impurity}$	Impurity $W_k \leftarrow \text{host}$ $R_k \leftarrow \text{impurity}$	$= u_{jk} + \left\{ -\frac{\Omega^2 m k_F}{12\pi^3 \hbar^3} \left(\frac{\nu_d \cdot R_j}{\nu_F}\right) \int_0^{2k_F} W_j(q) [W_j(q) - W_k(q)] q^3 dq \right\} + \left\{ -\frac{\Omega^2 m k_F}{4\pi^2 \hbar^2} \left(\frac{\nu_d}{\nu_F}\right) \cos(\nu_d, R_j - R_k) \times \int_0^{2k_F} W_j(q) [W_j(q) - W_k(q)] q^2 j_1(q R_j - R_k) dq \right\}$
Impurity $W_j \leftarrow \text{impurity}$ $R_j \leftarrow \text{impurity}$	Vacancy $W_k \leftarrow \text{host}$ $R_k \leftarrow \text{vacancy}$	$= u_{jk} + \left\{ -\frac{\Omega^2 m k_F}{12\pi^3 \hbar^3} \left(\frac{\nu_d \cdot R_j}{\nu_F}\right) \int_0^{2k_F} W_j(q) [W_j(q) - W_k(q)] q^3 dq \right\} - \left\{ -\frac{\Omega^2 m k_F}{4\pi^2 \hbar^2} \left(\frac{\nu_d}{\nu_F}\right) \cos(\nu_d, R_j - R_k) \times \int_0^{2k_F} W_j(q) W_k(q) q^2 j_1(q R_j - R_k) dq \right\}$

Results

The electromigration wind forces on substitutional impurities of several elements in aluminum were calculated with the use of Eq. (2) and are given in Table 3. Electromigration force directly depends on the electronic nature of the element, such that with the increased scattering power of the element an increase in the magnitude of the electromigration force was observed. In addition, the spatial distribution of the electromigration force nearby a vacancy and substitutional impurities were calculated in 2 dimensions. The force distribution nearby a vacancy, copper and titanium substitutional atoms can be seen in Figure 3(a), (b) and (c), respectively. The arrows indicate the direction of the force on each atom and the numbers give the scaled magnitude of the force. It can be seen that the magnitude of force on the atoms nearby the vacancy is quite high and aligned towards the applied drift. The distribution of the electromigration force in substitutional impurity systems varied depending on the electronic nature of the impurity element. The addition of Sn and Ti, for example, resulted in a negative force, in the opposite direction of the drift velocity, on the host atoms nearby the impurity, while the addition of Cu, Na, Mg and Mn caused a force distribution similar to the force

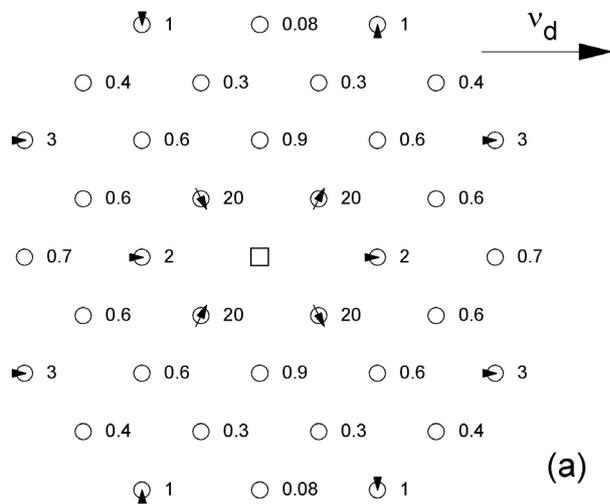


Figure 3. Spatial distribution of the electromigration forces on the (100) plane of the FCC lattice where (a) a vacancy, (b) copper and (c) titanium substitutional impurities were located at the center.

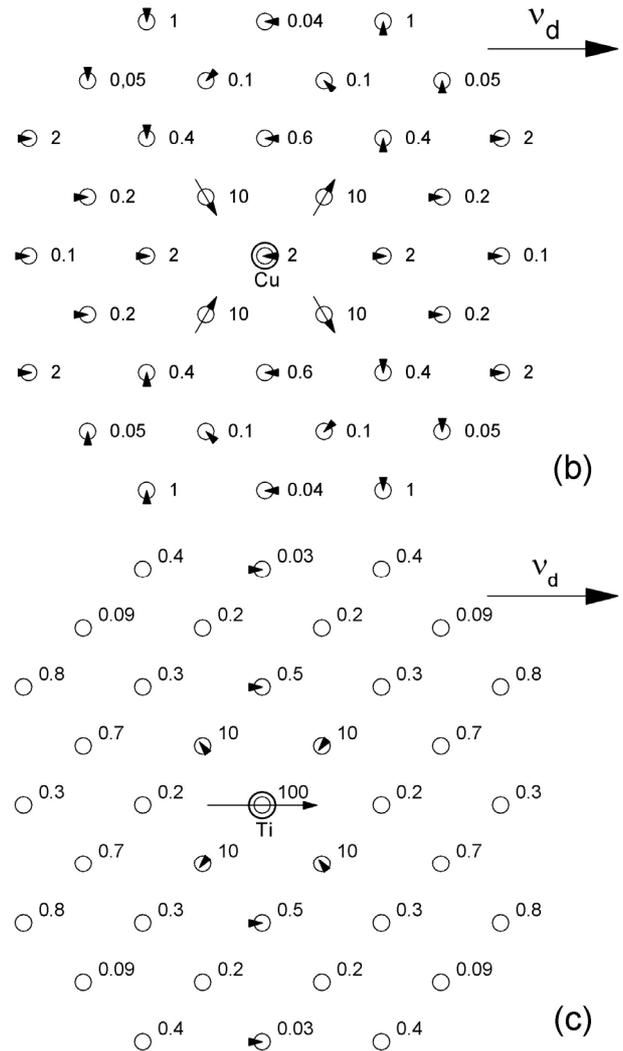


Figure 3. Continued.

distribution in the case of a vacancy. Additionally, except for Na, all alloying elements caused a decrease in the magnitudes of the forces on the host aluminum atoms compared to a vacancy. Much higher magnitudes of forces were calculated for the impurities of Ti and Sn atoms on themselves, and the forces were aligned along the direction of the drift velocity. The force calculated on Cu, however, was very small and it was aligned against the direction of the drift.

Table 3. Electromigration wind forces on elements that are added substitutionally to the aluminum with a drift velocity of 0.01 a.u. All forces are in eV/Å.

Element	Force	Element	Force	Element	Force	Element	Force
Li	0.00895	V	0.2944	Rb	0.196	Sn	0.0304
Be	0.0159	Cr	0.0362	Y	0.161	Sb	0.0901
B	0.1162	Mn	-0.0173	Zr	0.197	Te	0.1678
C	0.3169	Fe	0.0233	Nb	0.2128	Cs	0.2548
Na	0.0033	Co	-0.0143	Mo	0.2468	Ba	0.8022
Mg	-0.01024	Ni	-0.0144	Tc	0.1557	La	0.1086
Si	0.04903	Cu	-0.0018	Ru	0.1899	Hf	0.1413
P	0.1727	Zn	-0.0122	Rh	0.1518	Ta	0.1999
K	0.0938	Ga	0.0123	Pd	0.0024	W	0.2184
Ca	0.1141	Ge	0.0522	Ag	0.0152	Au	0.0941
Sc	0.0166	As	0.1535	Cd	0.0098	Pb	0.0425
Ti	0.1028	Se	0.2786	In	0.0137		

Table 4. Mean atomic jump frequencies ($\times 10^{-10}$ jumps/s) of the aluminum atoms in the systems investigated.

System / Temperature	1000 K	1200 K	1400 K
Al	12.236	18.580	23.693
Al - 1.125 at% Cu	3.952	10.169	24.031
Al - 1.125 at% Mg	9.125	16.012	30.825
Al - 1.125 at% Mn	5.254	21.518	29.960
Al - 1.125 at% Na	10.009	18.275	32.238
Al - 1.125 at% Sn	4.863	10.433	25.225
Al - 1.125 at% Ti	11.049	21.198	19.494

The incorporation of such calculated electron wind forces into the interatomic forces enabled the simulation of the diffusion process in a three-dimensional box under the effect of electromigration. However, because of the added force, which imposes non-equilibrium conditions, it is not possible to use equilibrium statistical mechanical descriptions of mean square displacement (MSD) or velocity autocorrelation function (VAF) for the understanding of the diffusivity phenomena. In addition, the approach suggested by Erpenbeck and Wood (1977) for the determination of the self-diffusion coefficient in non-equilibrium MD cannot be applied to our case, since it cannot handle multinary systems and, more importantly, the resulting diffusivity would be analogous to diffusivity computed in equilibrium MD, irrespective of the imposed electromigration force. Therefore, to characterize diffusion under electromigration forces, the description of the atomic jump frequency was used, in which for each atom in the box we measured the time required for it to jump from one lattice position to the other and how many times this happened. A successful jump was char-

acterized by a jump distance greater or equal to the nearest neighbor distance in the FCC lattice. Then the jump frequency, number of jumps per second, was averaged with respect to the number of atoms in the system. The above procedure was applied only to aluminum atoms in the system region, and the results are tabulated in Table 4 for the systems that we investigated.

As can be seen from Table 4, for all cases, except for Ti, jump frequency increases with the increased temperature as expected. In the case that aluminum was doped with Ti, there was a small decrease in the jump frequency of Al as temperature increased from 1200 to 1400 K. This behavior may be due to some inefficiency in the potential or some simulation parameters. In addition, for all impurities added, a decrease in the jump frequency of Al was observed. However, the amount of the decrease changes from impurity to impurity. At 1000 K, the most effective additions are Cu, Mn and Sn. Other elements, Mg, Na and Ti, were not so effective. For Cu, Mn and Sn, the jump frequency at 1000 K decreased respectively to 3.952×10^{-10} , to $5.254 \times$

10^{-10} and to 4.863×10^{-10} jumps per second, compared to jump frequency in pure Al, from 12.236×10^{-10} . As temperature increased, the above trend continued to hold except for Mn, where at 1200 K, for example, the jump frequency of Al in the Al-Mn alloy increased to 21.518×10^{-10} beyond the value of 18.58×10^{-10} in the pure Al. As temperature rose to 1400 K the system was so agitated that the effect of the alloying elements became less significant.

It is interesting to note that the impurity elements resulting in a decrease in the jump frequency have a softer character of pair potential with Al in common. Similarly, for the impurity elements having a softer potential character, the calculation of the electron wind force on the surrounding Al atoms resulted in lower magnitudes compared to the calculated force on Al atoms neighboring a vacancy in pure Al. This may be the reason for the decrease in the jump frequency in the alloys of those having soft Al-M pair potentials. However, although both Cu and Ti cause comparable electromigration forces developed at the surrounding Al atoms (see Figure 3), the diffusion characteristic of the alloys are totally different. Then the impurity element itself may play a role as well. Electromigration wind force on Cu, for example, was calculated to be very small,

whereas for Ti it was very large, meaning that Ti itself experiences a large disturbance due to electron scattering. This may cause agility in the surroundings as well. Therefore, compared to Cu, it may not cause a similar reduction in the diffusion kinetics of the Al atoms.

Therefore, diffusion of the host aluminum atoms seems to depend in a complicated way on how the electromigration and interatomic forces are developed, not only on aluminum atoms, but all over the constituent atoms.

Conclusions

It is shown in this study that incorporation of the electromigration force into molecular dynamics, within the necessities of the NEMD formalism, can be used to understand the diffusion process occurring in metallic alloys. The developed procedure was then applied to gain insight for the effect of alloying additions in aluminum alloys to be used as interconnects in integrated circuits. It is found that, when alloyed with aluminum, Cu, Mn and Sn reduced the kinetics of the atomic jumps. Cu is known experimentally to have such an effect on aluminum, but Mn and Sn are shown here for the first time to have a similar effect.

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